Berch 10_688606

09/13/2005

searched 1s attached

(structure

=> file registry FILE 'REGISTRY' ENTERED AT 10:13:08 ON 13 SEP 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 SEP 2005 HIGHEST RN 862971-50-4 DICTIONARY FILE UPDATES: 12 SEP 2005 HIGHEST RN 862971-50-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> file caplus FILE 'CAPLUS' ENTERED AT 10:13:30 ON 13 SEP 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 13 Sep 2005 VOL 143 ISS 12 FILE LAST UPDATED: 12 Sep 2005 (20050912/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate

substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> file uspatfull .

FILE 'USPATFULL' ENTERED AT 10:13:36 ON 13 SEP 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 8 Sep 2005 (20050908/PD)
FILE LAST UPDATED: 8 Sep 2005 (20050908/ED)
HIGHEST GRANTED PATENT NUMBER: US6941576
HIGHEST APPLICATION PUBLICATION NUMBER: US2005198721
CA INDEXING IS CURRENT THROUGH 8 Sep 2005 (20050908/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 8 Sep 2005 (20050908/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2005

>>> USPAT2 is now available. USPATFULL contains full text of the <<< >>> original, i.e., the earliest published granted patents or <<< >>> applications. USPAT2 contains full text of the latest US <<< >>> publications, starting in 2001, for the inventions covered in <<< >>> USPATFULL. A USPATFULL record contains not only the original <<< >>> published document but also a list of any subsequent <<< >>> publications. The publication number, patent kind code, and <<< >>> publication date for all the US publications for an invention <<< <<< >>> are displayed in the PI (Patent Information) field of USPATFULL >>> records and may be searched in standard search fields, e.g., /PN, <<< >>> /PK, etc. <<< <<< >>> USPATFULL and USPAT2 can be accessed and searched together <<< >>> through the new cluster USPATALL. Type FILE USPATALL to <<< >>> enter this cluster. <<< >>> >>> Use USPATALL when searching terms such as patent assignees, <<< <<< >>> classifications, or claims, that may potentially change from <<< >>> the earliest to the latest publication.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> file casreact FILE 'CASREACT' ENTERED AT 10:13:41 ON 13 SEP 2005 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE CONTENT:1840 - 11 Sep 2005 VOL 143 ISS 11

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

NODE ATT	KTF	BUTES	:		
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NSPEC	IS	R		ΑT	2
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NSPEC	IS	R		ΑT	4
NSPEC	IS	R		ΑT	5
NSPEC	IS	RC		ΑT	6
NSPEC	IS	R		ΑT	7
NSPEC	IS	R		ΑT	8
NSPEC	IS	С		ΑT	9
NSPEC	IS	С		ΑT	10
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NSPEC	IS	С		ΑT	20.
NSPEC	IS	RC		AT	21
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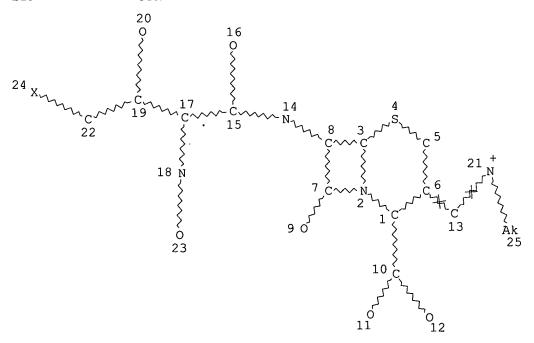
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CONNECT IS E3
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DEFAULT MLEVEL IS ATOM
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MLEVEL IS CLASS AT
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L17 49 SEA FILE=REGISTRY SSS FUL L15 L19 STR



NODE ATTRIBUTES:

CHARGE IS *+ AT 21 NSPEC IS R ΑT 2. NSPEC IS R ΑT 3 **NSPEC** IS R AT **NSPEC** IS R ΑT NSPEC IS R ΑT 5 IS RC NSPEC ΑT 7 **NSPEC** IS R ΑT NSPEC IS R ΑT 8 9 IS C NSPEC ΑT IS C 10 NSPEC ΑT NSPEC IS C AΤ 11 IS C 12 NSPEC AΤ IS RC 13 NSPEC ATIS C NSPEC AT14 NSPEC IS C AT15

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09/13/2005
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                   ΑT
                       16
NSPEC
        IS C
                   ΑT
                       17
        IS C
                       18
NSPEC
                   ΑT
        IS C
                       19
NSPEC
                   AΤ
                       20
NSPEC
        IS C
                   ΑT
NSPEC
        IS RC
                   ΑT
                       21
NSPEC
        IS C
                   ΑT
                       22
                       23
NSPEC
        IS C
                   AΤ
NSPEC
        IS C
                   AT
                       24
NSPEC
        IS C
                   AT
                       25
CONNECT IS E3
               RC AT
                        9
CONNECT IS E1
               RC AT
CONNECT IS E3
               RC AT
                       10
CONNECT IS E1
               RC AT
                       11
CONNECT IS E3
               RC AT
                       15
CONNECT IS E1
               RC AT
                       16
CONNECT IS E3
               RC AT
                       17
CONNECT IS E3
               RC AT
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DEFAULT MLEVEL IS ATOM
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MLEVEL IS CLASS AT
DEFAULT ECLEVEL IS LIMITED
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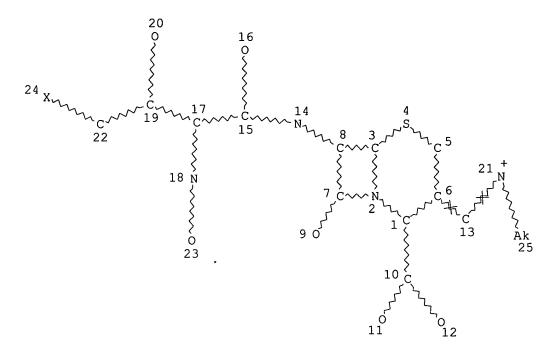
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

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                  AT
       IS R
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NSPEC
                       4
NSPEC
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                  ΑT
NSPEC
       IS R
                  ΑT
                       5
       IS RC
                       6
NSPEC
                  ΑT
                       7.
NSPEC
       IS R
                  AT
                       8
NSPEC
       IS R
                  AT
       IS C
                       9
NSPEC
                  AT
NSPEC
       IS C
                  AT
                      10
       IS C
                     11
NSPEC
                  AT
       IS C
NSPEC
                  AT
                     12
NSPEC
       IS RC
                  ΑT
                     13
NSPEC
       IS C
                  ΑT
                     14
NSPEC
       IS C
                  AT
                     15
NSPEC
       IS C
                  AT
                     16
NSPEC
       IS C
                  ΑT
                     17
NSPEC
       IS C
                  AΤ
                     18
       IS C
                  AΤ
                     19
NSPEC
       IS C
                  AT
                     20
NSPEC
NSPEC
       IS RC
                  ΑT
                      21
CONNECT IS E3
              RC AT
CONNECT IS E1
              RC AT
                      9
CONNECT IS E3
              RC AT
                      10
CONNECT IS E1
              RC AT
                      11
CONNECT IS E3
              RC AT
                      15
CONNECT IS E1
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                      16.
CONNECT IS E3
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                      17
CONNECT IS E3
              RC AT
                      19
CONNECT IS E1 RC AT
                      20
DEFAULT MLEVEL IS ATOM
                       9 10 11 12 13 14 15 16 17 18 19 20 21
MLEVEL IS CLASS AT
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 21
STEREO ATTRIBUTES: NONE
L17
             49 SEA FILE=REGISTRY SSS FUL L15
L19
                STR
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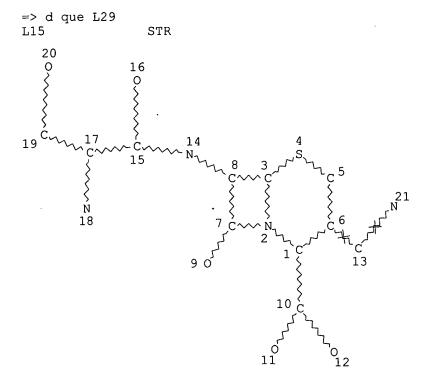
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NSPEC
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                    ΑT
                          4
5
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                    AT
                          6
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                    AT
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                    AT
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                    AT
                         11
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                    ΑT
                         12
NSPEC
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                    ΑT
                         13
NSPEC
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                    ΑT
                         14
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        IS C
                    AT
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        IS C
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NSPEC
                         25
NSPEC
        IS C
                    ΑT
CONNECT IS E3
                         7
                RC AT
                RC AT
                          9
CONNECT IS E1
CONNECT IS E3
                RC AT
                         10
CONNECT IS E1
                RC AT
                         11
CONNECT IS E3
                RC AT
                         15
CONNECT IS E1
                RC AT
                         16
CONNECT IS E3
                RC AT
                         17.
```

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CONNECT IS E3 RC AT 19
CONNECT IS E1 RC AT 20
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
DEFAULT ECLEVEL IS LIMITED
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RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L22 8 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L28 2 SEA L22 USPATFULL, CASREACT hits



NODE AT	TRI	BUTES:		
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NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AΤ	4
NSPEC	IS	R	AT	5
NSPEC	IS	RC	AT	6
NSPEC	IS	R	AT	7*
NSPEC	IS	R	ΑT	8
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NSPEC	IS	С	AT	11
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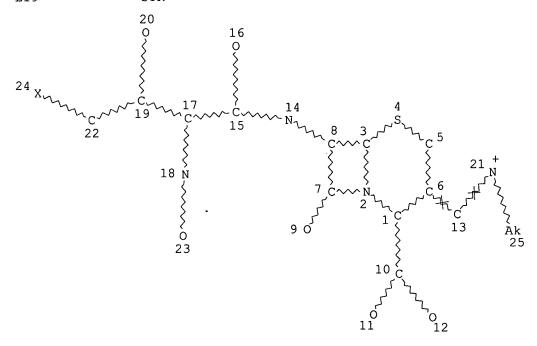
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                       18
NSPEC
                   AT
        IS C
                   AT
                       19
NSPEC
        IS C
                   ΑT
                       20
NSPEC
NSPEC
        IS RC
                   AT
                       21
CONNECT IS E3
               RC AT
                        7
                        9
CONNECT IS E1
               RC AT
CONNECT IS E3
               RC AT
                       10
CONNECT IS E1
               RC AT
                       11
CONNECT IS E3
               RC AT
                       15
CONNECT IS E1
               RC AT
                       16
                       17
CONNECT IS E3
               RC AT
CONNECT IS E3
               RC AT
                       19
CONNECT IS E1
               RC AT
                       20
DEFAULT MLEVEL IS ATOM
                        9 10 11 12 13 14 15 16 17 18 19 20 21
MLEVEL IS CLASS AT
DEFAULT ECLEVEL IS LIMITED
```

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L17 49 SEA FILE=REGISTRY SSS FUL L15 L19 STR



NODE ATTRIBUTES:

CHARGE	IS	*+	AT	21
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NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	RC	AT	6
NSPEC	IS	R	AT	7

```
AT
NSPEC
      IS R
                    8
NSPEC IS C
                  9
              AΤ
NSPEC IS C
              AT 10
NSPEC IS C
              AT 11
NSPEC IS C
              AT 12
NSPEC IS RC
              AT 13
NSPEC IS C
              AT 14
NSPEC IS C
              AT 15
NSPEC IS C
              AT 16
NSPEC IS C
              AT 17
NSPEC IS C
              AT 18.
NSPEC IS C
              AT 19
NSPEC IS C
              AT 20
NSPEC IS RC
              AT 21
NSPEC IS C
               AT 22
NSPEC IS C
               AT 23
NSPEC IS C
               AT 24
NSPEC IS C
               AT 25
CONNECT IS E3 RC AT
                   7
                   9
CONNECT IS E1 RC AT
CONNECT IS E3 RC AT 10
CONNECT IS E1 RC AT 11
CONNECT IS E3 RC AT 15
CONNECT IS E1 RC AT 16
CONNECT IS E3 RC AT
                  17
CONNECT IS E3 RC AT
                  19
CONNECT IS E1 RC AT
                   20
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
                    9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
DEFAULT ECLEVEL IS LIMITED
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RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L22 8 SEA FILE=REGISTRY SUB=L17 SSS FUL L19 L23 2 SEA FILE=CAPLUS ABB=ON PLU=ON L22

L28 2 SEA L22

L29 2 DUP REM L23 L28 (2 DUPLICATES REMOVED)

=> file stnguide

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Sep 9, 2005 (20050909/UP).

=> d ibib abs hitstr L29 1-2

YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L29 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2005:160883 CAPLUS

DOCUMENT NUMBER: 142:261334

TITLE:

Process for preparing cefepime by the

cyclocondensation reaction of thiourea with a

brominated or chlorinated derivative

INVENTOR(S):

Handa, Vijay Kumar; Kamat, Anand G.; Sivakumaran,

Meenakshisunderam

PATENT ASSIGNEE(S):

India

SOURCE:

U.S. Pat. Appl. Publ., 5 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

KIND DATE ____

APPLICATION NO

DATE

------US 2005043531

20050224 Α1

US 2003-688606 IN 2003-CH669

20031017 20030821

This work

PRIORITY APPLN. INFO.:

OTHER SOURCE(S):

PATENT NO.

CASREACT 142:261334

GI

OMe N CO-NH CH3 C00-

Cefepime, a cephalosporin antibiotic, is prepared in high yield and AB selectivity by the cyclocondensation of thiourea with bromo or chloro derivative I (X = Br, Cl) which is prepared by the amidation of 7-amino-3-[(1-methyl-1-pyrrolidinium)methyl]-3-cephem-4-carboxylate with a corresponding 4-halo-2-methoxyimino-3-oxobutyric acid halide. Thus, cefepime dihydrochloride monohydrate was prepared from 7-amino-3-[(1-methyl-1-pyrrolidinium)methyl]-3-cephem-4-carboxylate hydrochloride via silylation with Me3SiNHAc in CH2Cl2, acylation with freshly prepared 4-bromo-2-methoxyimino-3-oxobutyryl chloride in CH2Cl2 and cyclocondensation of intermediate I (X = Br) with H2NC(:S)NH2 in aqueous MeCOMe.

Ι

846021-46-3P 846021-47-4P 846021-48-5P IT

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in a process for preparing cefepime by the cyclocondensation reaction of thiourea with a brominated or chlorinated derivative)

RN 846021-46-3 CAPLUS

Pyrrolidinium, 1-[[(6R,7R)-2-carboxy-7-[[4-chloro-2-(methoxyimino)-1,3-CN dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1methyl-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 846021-47-4 CAPLUS.

CN Pyrrolidinium, 1-[[(6R,7R)-7-[[4-bromo-2-(methoxyimino)-1,3-dioxobutyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

● Cl -

RN 846021-48-5 CAPLUS

CN Pyrrolidinium, 1-[[(6R,7R)-2-carboxy-7-[[4-chloro-2-(methoxyimino)-1,3-dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

● C1-

IT 846021-45-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (process for preparing cefepime by the cyclocondensation reaction of thiourea with a brominated or chlorinated derivative)

RN 846021-45-2 CAPLUS

CN Pyrrolidinium, 1-[['(6R,7R)-7-[[4-bromo-2-(methoxyimino)-1,3-dioxobutyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

L29 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:902392 CAPLUS

DOCUMENT NUMBER: 141:366239

TITLE: A preparation of antibacterial 5-thia-1-

azabicyclo[4.2.0]octane derivative (cefepime)

INVENTOR(S): Ludescher, Johannes; Sturm, Hubert; Wolf, Siegfried

PATENT ASSIGNEE(S): Sandoz A.-G., Switz. SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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WO 2004-EP3988
                          A2
                                20041028
                                                                    20040415
    WO 2004092183
                                20041209
    WO 2004092183
                         A3
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
        W:
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
            ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
            SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
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                                            AT 2003-584
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PRIORITY APPLN. INFO.:
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                                                                    20030416
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OTHER SOURCE(S): GΙ

MARPAT 141:366239

Me

CO2:

The invention relates to a preparation of 5-thia-1-azabicyclo[4.2.0] octane AΒ derivative I (cefepime), useful as antibacterial agent (no biol. data). For instance, 5-thia-1-azabicyclo[4.2.0]octane derivative (I•2HCl) was prepared via heterocyclization of chloro(methoxyimino)oxobutyric acid derivative II-HCl and thiourea (example 3, 99.6% of purity).

Ι

ΙT 780810-16-4P 780810-18-6P

> RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of antibacterial cefepime from thiaazabicyclo[4.2.0]octane derivs. and thiourea)

RN 780810-16-4 CAPLUS-

Pyrrolidinium, 1-[[(6R,7R)-2-carboxy-7-[[(2Z)-4-chloro-2-(methoxyimino)-CN 1,3-dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3yl]methyl]-1-methyl-, inner salt, monohydrochloride (9CI) (CA INDEX NAME) Absolute stereochemistry. Double bond geometry as shown.

● HCl

RN 780810-18-6 CAPLUS

CN Pyrrolidinium, 1-[[(6R,7R)-2-carboxy-7-[[(2Z)-4-chloro-2-(methoxyimino)-1,3-dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Beilstein search on narrower (reguested)

Berch 10_688606 Structure 09/13/2005

=> file beilstein FILE 'BEILSTEIN' ENTERED AT 10:23:30 ON 13 SEP 2005 COPYRIGHT (c) 2005 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002 FILE LAST UPDATED ON JUNE 29, 2005

FILE COVERS 1771 TO 2005. *** FILE CONTAINS 9,271,550 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<

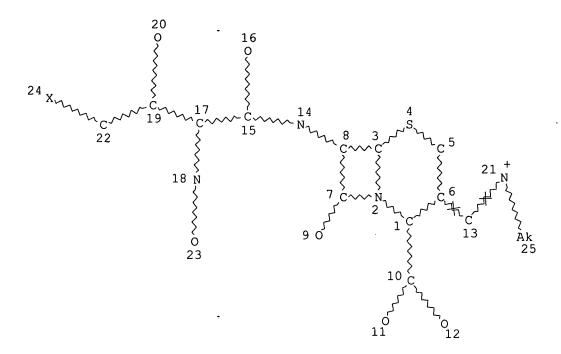
>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

- * PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.
- * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE
- * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE
- * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.
- * FOR PRICE INFORMATION SEE HELP COST

NEW

- * PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
- * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> d stat que L30 L19 STR



```
NODE ATTRIBUTES:
CHARGE
        IS *+
                    AT
                         21
NSPEC
         IS R
                    ΑT
                          1
                          2
         IS R
                    ΑT
NSPEC
                          3
         IS R
                    ΑT
NSPEC
                          4
         IS R
NSPEC
                    ΑT
                          5
NSPEC
         IS R
                    ΑT
                          6
NSPEC
         IS RC
                    AT
                          7
         IS R
                    AT
NSPEC
                          8
         IS R
                    ΑT
NSPEC
                          9
         IS C
                    ΑT
NSPEC
         IS C
                    ΑT
                         10
NSPEC
NSPEC
         IS C
                    ΑT
                         11
NSPEC
         IS C
                    AΤ
                         12
NSPEC
         IS RC
                    ΑT
                         13
         IS C
                         14
NSPEC
                    ΑT
         IS C
NSPEC
                    AΤ
                         15
         IS C
                         16
NSPEC
                    AΤ
NSPEC
         IS C
                    AT
                         17
         IS C
                    AT
                         18
NSPEC
                         19
         IS C
                    ΑT
NSPEC
                         20
         IS C
                    ΑT
NSPEC
         IS RC
                    ΑT
                         21
NSPEC
                         22
NSPEC
         IS C
                    ΑT
         IS C
                    ΑT
                         23
NSPEC
         IS C
                    ΑT
                         24
NSPEC
                         25
NSPEC
         IS C
                    AΤ
                          7
CONNECT IS E3
                 RC AT
CONNECT IS E1
                 RC AT
                          9
                         10
CONNECT IS E3
                 RC AT
CONNECT IS E1
                 RC AT
                         11
                         15
CONNECT IS E3
                 RC AT
CONNECT IS E1
                 RC AT
                         16
CONNECT IS E3
                 RC AT
                         17
```

CONNECT IS E3 RC AT 19
CONNECT IS E1 RC AT 20
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

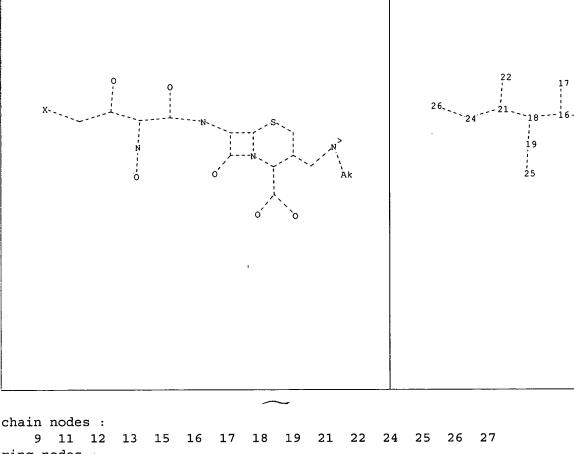
STEREO ATTRIBUTES: NONE

L30 0 SEA FILE=BEILSTEIN SSS FUL L19

100.0% PROCESSED 84 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.04

C:\Program Files\Stnexp\Queries\10_688606\ber-i.str_



9 11 12 13 15 16 17 18 19 21 22 24 25 26 27

ring nodes:

1 2 3 4 5 6 7 8

ring/chain nodes:

14 23

chain bonds:

1-11 7-9 8-15 11-12 11-13 15-16 16-17 16-18 18-19 18-21 19-25 21-22 21-24

23-27 24-26

ring/chain bonds:

6-14 14-23

ring bonds:

1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8

exact/norm bonds:

1-2 1-6 1-11 2-3 2-7 3-4 3-8 4-5 5-6 6-14 7-8 7-9 8-15 11-12 11-13 14-23

15-16 16-17 16-18 18-19 18-21 19-25 21-22 21-24 23-27 24-26

Connectivity :

7:3 E exact RC ring/chain 9:1 E exact RC ring/chain 11:3 E exact RC ring/chain 12:1 E exact RC ring/chain 16:3 E exact RC ring/chain 17:1 E exact RC ring/chain 18:3 E exact RC ring/chain 21:3 E exact RC ring/chain 22:1 E exact RC ring/chain Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS

structure L15 C:\Program Files\Stnexp\Queries\10 688606\ber-h.str__ chain nodes :

```
9 11 12 13 15 16 17 18 19 21 22

ring nodes :
    1 2 3 4 5 6 7 8

ring/chain nodes :
    14 23

chain bonds :
    1-11 7-9 8-15 11-12 11-13 15-16 16-17 16-18 18-19 18-21 21-22

ring/chain bonds :
    6-14 14-23

ring bonds :
    1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8

exact/norm bonds :
    1-2 1-6 1-11 2-3 2-7 3-4 3-8 4-5 5-6 6-14 7-8 7-9 8-15 11-12 11-13 14-23

15-16 16-17 16-18 18-19 18-21 21-22
```

Connectivity :

7:3 E exact RC ring/chain 9:1 E exact RC ring/chain 11:3 E exact RC ring/chain 12:1 E exact RC ring/chain 16:3 E exact RC ring/chain 17:1 E exact RC ring/chain 18:3 E exact RC ring/chain 21:3 E exact RC ring/chain 22:1 E exact RC ring/chain Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS